W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 07:30 PM GMT

PDB ID	:	1H3X
Title	:	CRYSTAL STRUCTURE OF THE HUMAN IGG1 FC-FRAGMENT,GLYCOFORM(G0F)2
Authors	:	Krapp, S.; Mimura, Y.; Jefferis, R.; Huber, R.; Sondermann, P.
Deposited on	:	2002-09-19
Resolution	:	2.44 Å(reported)

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.328
Clashscore		36
Ramachandran outliers		5.1%
Sidechain outliers		4.7%
RSRZ outliers		8.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
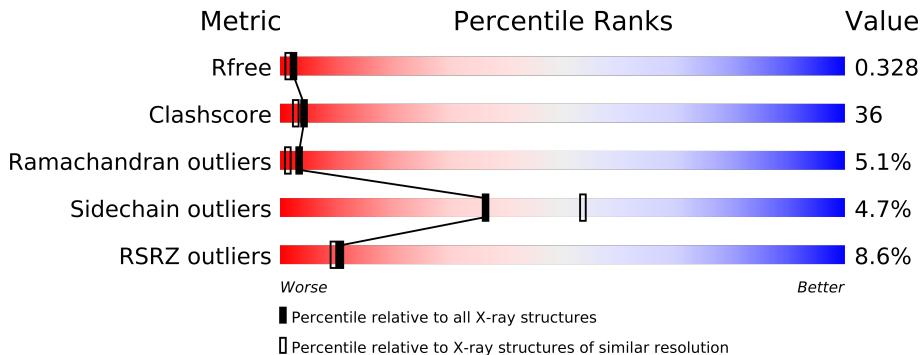
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2989 (2.48-2.40)
Clashscore	79885	3698 (2.48-2.40)
Ramachandran outliers	78287	3639 (2.48-2.40)
Sidechain outliers	78261	3640 (2.48-2.40)
RSRZ outliers	66119	2993 (2.48-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	223	
1	B	223	
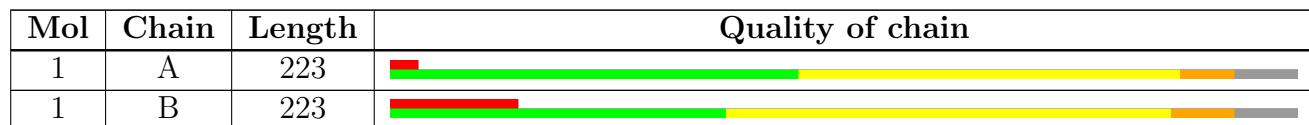
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3668 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IG GAMMA-1 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total 1661	C 1057	N 283	O 314	S 7	0	0	1
1	B	207	Total 1655	C 1054	N 281	O 313	S 7	0	0	1

- Molecule 2 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	8	Total 99	C 56	N 4	O 39	0	0
2	B	8	Total 99	C 56	N 4	O 39	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total 75	O 75	0	0
3	B	79	Total 79	O 79	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
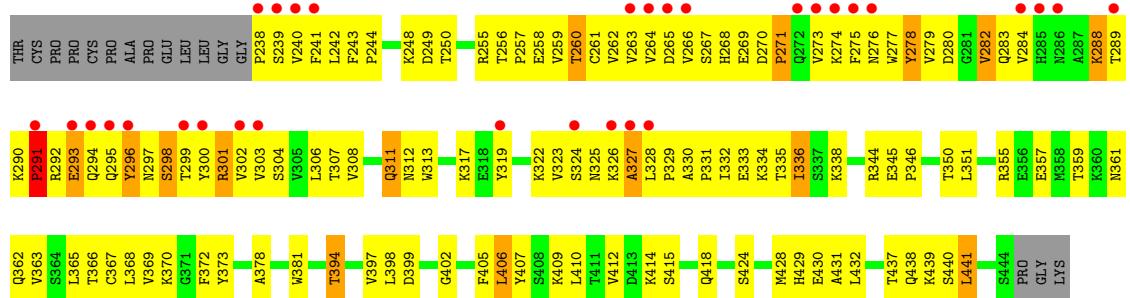
- Molecule 1: IG GAMMA-1 CHAIN C REGION

Chain A:
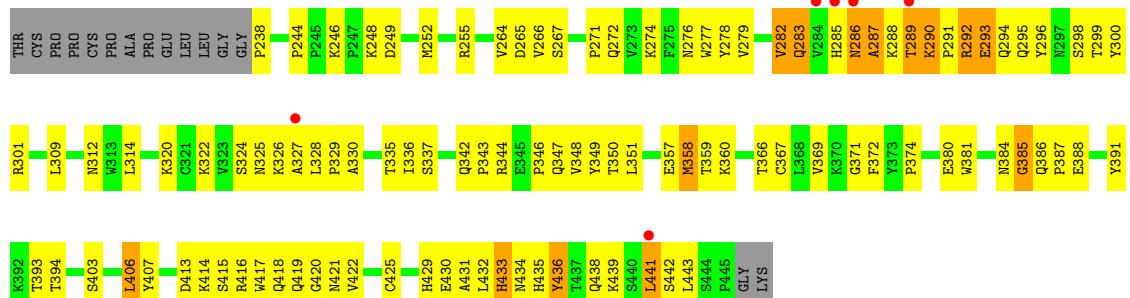
- Molecule 1: IG GAMMA-1 CHAIN C REGION

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	49.69Å 80.20Å 138.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.44 40.42 – 2.45	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-2.44) 93.8 (40.42-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 2.45Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.278 , 0.339 0.280 , 0.328	Depositor DCC
R_{free} test set	961 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.42, < L^2 > = 0.25$	Xtriage
Outliers	0 of 19884 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3668	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.44	0/1707	0.68	0/2325
1	B	0.38	0/1700	0.64	0/2314
All	All	0.41	0/3407	0.66	0/4639

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	B	1	0
All	All	1	1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1451	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	373	TYR	Sidechain

5.2 Close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1661	0	1631	109	0
1	B	1655	0	1625	133	0
2	A	99	0	85	4	0
2	B	99	0	85	14	0
3	A	75	0	0	13	0
3	B	79	0	0	14	0
All	All	3668	0	3426	252	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (252) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:1444:NAG:H61	2:B:1446:NAG:HN2	1.05	1.19
2:B:1444:NAG:H61	2:B:1446:NAG:N2	1.79	0.98
1:B:266:VAL:HB	1:B:300:TYR:HB2	1.44	0.96
1:A:272:GLN:HE22	1:A:326:LYS:HD2	1.35	0.92
1:B:311:GLN:NE2	1:B:311:GLN:H	1.71	0.87
1:A:282:VAL:O	1:A:283:GLN:HB2	1.72	0.87
1:B:328:LEU:HD21	1:B:332:ILE:HG13	1.59	0.84
1:B:243:PHE:HB2	1:B:260:THR:HG23	1.60	0.84
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.60	0.83
1:B:291:PRO:HB3	1:B:304:SER:HA	1.60	0.82
1:B:346:PRO:HB3	1:B:372:PHE:HB3	1.63	0.80
1:A:314:LEU:HD22	1:A:430:GLU:HG3	1.62	0.79
1:B:289:THR:HG22	1:B:290:LYS:H	1.48	0.79
1:B:263:VAL:O	1:B:301:ARG:HA	1.84	0.78
2:B:1448:MAN:O5	2:B:1449:NAG:H82	1.81	0.78
1:A:291:PRO:C	1:A:292:ARG:HD2	2.03	0.78
1:A:292:ARG:O	1:A:293:GLU:HB3	1.84	0.76
1:B:429:HIS:CD2	1:B:431:ALA:H	2.03	0.76
1:B:266:VAL:HB	1:B:300:TYR:CB	2.15	0.75
1:A:429:HIS:CD2	1:A:431:ALA:H	2.05	0.75
1:A:296:TYR:CD2	2:A:1446:FUL:H2	2.22	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:GLN:NE2	1:A:326:LYS:HD2	2.01	0.74
1:B:429:HIS:HD2	1:B:431:ALA:H	1.31	0.74
2:B:1444:NAG:C6	2:B:1446:NAG:HN2	1.94	0.73
1:B:328:LEU:HD12	1:B:329:PRO:HD2	1.69	0.73
1:B:365:LEU:HD12	1:B:410:LEU:HD23	1.69	0.72
1:B:296:TYR:HE2	2:B:1444:NAG:H62	1.53	0.72
1:B:296:TYR:CE2	2:B:1444:NAG:H62	2.24	0.72
1:B:288:LYS:H	1:B:288:LYS:HD3	1.54	0.71
1:B:409:LYS:HE2	3:B:2041:HOH:O	1.92	0.69
1:A:422:VAL:HG22	1:A:442:SER:OG	1.92	0.68
1:B:270:ASP:N	1:B:271:PRO:HD3	2.09	0.68
1:A:325:ASN:HD21	1:A:327:ALA:HB3	1.58	0.68
1:A:252:MET:HB2	1:A:255:ARG:HG3	1.75	0.68
1:A:418:GLN:HA	1:A:443:LEU:CD2	2.24	0.68
1:A:429:HIS:HD2	1:A:431:ALA:H	1.43	0.67
1:A:325:ASN:ND2	1:A:327:ALA:HB3	2.10	0.67
1:B:290:LYS:HE3	1:B:292:ARG:HH22	1.61	0.66
2:A:1447:NAG:H83	2:A:1449:MAN:O4	1.96	0.66
1:A:350:THR:HB	1:A:441:LEU:HG	1.77	0.65
1:B:439:LYS:HB2	3:B:2034:HOH:O	1.96	0.64
1:B:332:ILE:HG22	1:B:333:GLU:N	2.13	0.64
1:A:328:LEU:HG	1:A:330:ALA:O	1.98	0.64
1:A:288:LYS:H	1:A:288:LYS:HD2	1.63	0.63
1:A:279:VAL:O	1:A:282:VAL:HG13	1.97	0.63
1:B:330:ALA:HB1	1:B:331:PRO:HD2	1.79	0.63
1:B:258:GLU:HB3	3:B:2017:HOH:O	1.98	0.63
1:B:409:LYS:HG2	3:B:2067:HOH:O	1.98	0.63
2:B:1450:MAN:H4	2:B:1451:NAG:O7	1.98	0.63
1:A:384:ASN:O	1:A:386:GLN:N	2.31	0.63
1:B:355:ARG:HD2	3:B:2038:HOH:O	2.00	0.62
1:A:300:TYR:HA	3:A:2020:HOH:O	1.99	0.61
1:B:394:THR:HG23	1:B:407:TYR:O	2.01	0.60
1:B:406:LEU:C	1:B:406:LEU:HD12	2.22	0.60
1:B:274:LYS:HE2	1:B:276:ASN:HD21	1.67	0.60
1:B:325:ASN:HD22	1:B:326:LYS:H	1.51	0.59
1:B:267:SER:HA	3:B:2007:HOH:O	2.02	0.59
1:A:417:TRP:HH2	1:A:441:LEU:HD22	1.67	0.59
1:B:269:GLU:HG2	1:B:269:GLU:O	2.03	0.58
1:A:417:TRP:CH2	1:A:441:LEU:HD22	2.37	0.58
1:A:276:ASN:HB2	1:A:322:LYS:HB3	1.85	0.58
1:A:286:ASN:O	1:A:287:ALA:HB2	2.03	0.58
1:B:296:TYR:CE1	1:B:301:ARG:HD3	2.38	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:279:VAL:O	1:B:279:VAL:HG23	2.03	0.58
1:A:433:HIS:ND1	1:A:434:ASN:OD1	2.36	0.58
1:A:415:SER:O	1:A:419:GLN:HG3	2.04	0.58
1:A:421:ASN:N	1:A:421:ASN:HD22	2.00	0.58
1:B:424:SER:OG	1:B:438:GLN:HG2	2.04	0.58
1:B:257:PRO:HB2	1:B:308:VAL:HB	1.85	0.57
1:A:344:ARG:HG2	3:A:2035:HOH:O	2.04	0.57
1:B:265:ASP:HA	1:B:299:THR:HB	1.86	0.57
1:B:288:LYS:HE2	1:B:306:LEU:HD11	1.86	0.57
1:B:439:LYS:HE3	1:B:440:SER:O	2.05	0.56
1:A:320:LYS:HG3	1:A:335:THR:HG22	1.87	0.56
1:B:328:LEU:HG	1:B:330:ALA:O	2.05	0.56
1:B:301:ARG:HE	1:B:303:VAL:CG2	2.18	0.56
1:B:311:GLN:CD	1:B:311:GLN:H	2.08	0.56
1:B:325:ASN:ND2	1:B:326:LYS:H	2.04	0.55
1:B:270:ASP:OD2	1:B:327:ALA:HB2	2.06	0.55
1:A:328:LEU:HD12	1:A:329:PRO:HD2	1.88	0.55
1:B:241:PHE:CE2	2:B:1447:BMA:H3	2.42	0.55
1:B:273:VAL:HG13	3:B:2011:HOH:O	2.07	0.55
1:B:275:PHE:HE1	1:B:302:VAL:HG12	1.72	0.55
1:B:266:VAL:CB	1:B:300:TYR:HB2	2.28	0.54
1:A:289:THR:O	1:A:290:LYS:HB2	2.07	0.54
1:B:240:VAL:O	1:B:334:LYS:HE3	2.08	0.54
1:A:288:LYS:O	1:A:289:THR:O	2.24	0.54
1:B:238:PRO:CG	1:B:328:LEU:HD13	2.37	0.54
2:B:1448:MAN:C1	2:B:1449:NAG:H82	2.37	0.54
1:A:414:LYS:HE2	1:A:418:GLN:NE2	2.22	0.54
1:B:351:LEU:C	1:B:441:LEU:HD11	2.28	0.54
1:A:414:LYS:O	1:A:418:GLN:HG3	2.08	0.54
1:A:300:TYR:HD2	3:A:2011:HOH:O	1.91	0.53
1:A:282:VAL:O	1:A:283:GLN:CB	2.52	0.53
1:A:285:HIS:O	1:A:286:ASN:HB2	2.08	0.53
1:B:322:LYS:HE3	1:B:333:GLU:OE2	2.08	0.53
1:B:262:VAL:HG13	1:B:303:VAL:HG22	1.90	0.53
1:A:296:TYR:HD2	2:A:1446:FUL:H2	1.72	0.53
1:B:289:THR:HG22	1:B:290:LYS:N	2.21	0.52
1:A:418:GLN:HA	1:A:443:LEU:HD22	1.90	0.52
1:B:312:ASN:ND2	1:B:317:LYS:HD2	2.24	0.52
1:A:351:LEU:HB2	1:A:366:THR:HB	1.90	0.52
1:A:384:ASN:OD1	1:A:385:GLY:N	2.41	0.52
1:A:393:THR:HG22	1:A:394:THR:O	2.10	0.52
1:A:337:SER:HB2	3:A:2027:HOH:O	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1452:NAG:H83	2:A:1452:NAG:O3	2.09	0.52
1:B:297:ASN:O	1:B:298:SER:HB3	2.09	0.52
1:B:296:TYR:HE1	1:B:301:ARG:HD3	1.74	0.52
1:A:271:PRO:HD2	3:A:2013:HOH:O	2.08	0.52
1:B:249:ASP:O	1:B:257:PRO:HG3	2.10	0.52
2:B:1450:MAN:HO3	2:B:1451:NAG:C1	2.23	0.52
1:B:325:ASN:ND2	1:B:326:LYS:N	2.59	0.51
1:A:429:HIS:O	1:A:435:HIS:HA	2.11	0.51
1:A:350:THR:HB	1:A:441:LEU:CG	2.40	0.51
1:A:436:TYR:C	1:A:436:TYR:CD1	2.84	0.51
1:A:418:GLN:C	1:A:420:GLY:H	2.15	0.50
1:A:443:LEU:HG	1:A:443:LEU:O	2.11	0.50
1:B:378:ALA:HB3	1:B:428:MET:HB2	1.92	0.50
1:B:291:PRO:CB	1:B:304:SER:HA	2.37	0.50
1:A:294:GLN:O	1:A:300:TYR:CD1	2.65	0.50
1:B:406:LEU:HD12	1:B:406:LEU:O	2.12	0.50
1:A:380:GLU:O	1:A:425:CYS:HA	2.12	0.50
1:A:360:LYS:O	1:A:414:LYS:HD2	2.11	0.50
1:B:332:ILE:CG2	1:B:333:GLU:N	2.74	0.50
1:B:249:ASP:C	1:B:257:PRO:HG3	2.32	0.50
1:A:246:LYS:HB2	1:A:249:ASP:OD2	2.12	0.50
1:B:369:VAL:O	1:B:405:PHE:HA	2.12	0.50
1:A:292:ARG:O	1:A:293:GLU:CB	2.58	0.49
1:A:299:THR:HA	3:A:2011:HOH:O	2.11	0.49
1:B:278:TYR:CD1	1:B:278:TYR:N	2.79	0.49
1:B:291:PRO:HB3	1:B:304:SER:CA	2.37	0.49
1:A:248:LYS:O	1:A:255:ARG:HD3	2.13	0.49
1:B:250:THR:HG22	1:B:257:PRO:HB3	1.94	0.49
1:A:357:GLU:C	1:A:359:THR:H	2.15	0.49
1:B:256:THR:HG23	3:B:2003:HOH:O	2.12	0.49
1:A:388:GLU:OE2	1:A:416:ARG:NH2	2.42	0.49
1:A:277:TRP:O	1:A:283:GLN:HB3	2.13	0.49
1:B:292:ARG:O	1:B:293:GLU:HB3	2.12	0.49
1:B:432:LEU:CD1	1:B:437:THR:HG22	2.42	0.48
1:A:278:TYR:HB2	1:A:320:LYS:HB3	1.94	0.48
1:A:283:GLN:C	1:A:285:HIS:N	2.63	0.48
1:A:346:PRO:CB	1:A:372:PHE:HB3	2.39	0.48
1:A:301:ARG:N	3:A:2020:HOH:O	2.46	0.48
1:B:259:VAL:HG23	1:B:308:VAL:CG2	2.43	0.48
1:B:274:LYS:N	3:B:2011:HOH:O	2.44	0.48
1:B:261:CYS:HB2	1:B:277:TRP:CZ2	2.47	0.48
1:B:312:ASN:HB3	1:B:319:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:238:PRO:HD3	3:A:2001:HOH:O	2.14	0.48
1:A:266:VAL:O	1:A:300:TYR:HB2	2.13	0.48
1:A:358:MET:O	1:A:414:LYS:HE3	2.14	0.47
1:B:275:PHE:HZ	1:B:302:VAL:O	1.97	0.47
1:A:388:GLU:HA	1:A:388:GLU:OE1	2.14	0.47
1:B:244:PRO:HB3	1:B:336:ILE:HD11	1.95	0.47
1:A:414:LYS:HG2	1:A:418:GLN:NE2	2.29	0.47
1:B:398:LEU:HD11	1:B:402:GLY:HA2	1.95	0.47
1:A:371:GLY:HA2	1:A:403:SER:OG	2.14	0.47
2:B:1444:NAG:O6	2:B:1445:FUL:H63	2.14	0.47
1:A:289:THR:CG2	1:A:290:LYS:N	2.78	0.47
1:A:283:GLN:CD	1:A:287:ALA:HB2	2.34	0.47
1:B:248:LYS:HD2	3:B:2051:HOH:O	2.15	0.47
1:B:296:TYR:HB3	1:B:297:ASN:H	1.34	0.47
1:B:368:LEU:HD12	1:B:369:VAL:H	1.79	0.47
1:A:438:GLN:O	1:A:439:LYS:HD3	2.15	0.47
1:B:350:THR:HB	1:B:441:LEU:HG	1.95	0.47
1:A:288:LYS:H	1:A:288:LYS:CD	2.27	0.47
1:A:380:GLU:HB3	3:A:2047:HOH:O	2.14	0.46
1:B:261:CYS:HB2	1:B:277:TRP:CH2	2.50	0.46
1:B:361:ASN:ND2	1:B:362:GLN:HG3	2.31	0.46
1:A:286:ASN:O	1:A:287:ALA:CB	2.63	0.46
1:B:278:TYR:CE2	1:B:284:VAL:HG22	2.50	0.46
1:B:279:VAL:O	1:B:282:VAL:HG22	2.15	0.46
1:B:432:LEU:HD22	1:B:437:THR:HB	1.97	0.46
1:B:322:LYS:HG3	1:B:333:GLU:HG2	1.97	0.46
1:B:432:LEU:HD11	1:B:437:THR:HG22	1.98	0.46
1:B:294:GLN:NE2	3:B:2016:HOH:O	2.46	0.46
1:B:308:VAL:HG11	1:B:313:TRP:HB2	1.97	0.46
1:A:295:GLN:HA	3:A:2020:HOH:O	2.15	0.46
1:B:344:ARG:O	1:B:372:PHE:HA	2.16	0.46
1:A:296:TYR:HD1	3:A:2020:HOH:O	1.97	0.46
1:B:300:TYR:O	1:B:301:ARG:CB	2.64	0.45
1:B:300:TYR:O	1:B:301:ARG:HB2	2.16	0.45
1:B:345:GLU:HA	1:B:431:ALA:HB3	1.98	0.45
1:A:278:TYR:CD1	1:A:278:TYR:N	2.85	0.45
1:B:242:LEU:HD13	1:B:336:ILE:HG22	1.98	0.45
1:B:269:GLU:C	1:B:271:PRO:HD3	2.36	0.45
1:A:374:PRO:O	1:A:429:HIS:HE1	2.00	0.45
1:B:238:PRO:CB	1:B:328:LEU:HD13	2.47	0.45
1:A:265:ASP:HA	1:A:299:THR:HB	1.98	0.45
1:A:421:ASN:N	1:A:421:ASN:ND2	2.64	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:326:LYS:C	1:B:328:LEU:H	2.20	0.45
1:B:406:LEU:C	1:B:406:LEU:CD1	2.84	0.45
1:B:290:LYS:HE3	1:B:292:ARG:HH12	1.82	0.45
1:A:244:PRO:HB3	1:A:336:ILE:HD13	1.99	0.45
1:B:415:SER:HB3	3:B:2068:HOH:O	2.17	0.44
1:B:323:VAL:HG12	1:B:324:SER:N	2.32	0.44
1:A:291:PRO:O	1:A:292:ARG:HD2	2.17	0.44
1:A:347:GLN:NE2	1:A:349:TYR:OH	2.50	0.44
1:B:239:SER:HB3	1:B:264:VAL:CG2	2.47	0.44
1:B:258:GLU:HA	1:B:308:VAL:HG23	1.99	0.44
1:B:279:VAL:O	1:B:280:ASP:HB2	2.17	0.44
1:A:309:LEU:O	1:A:312:ASN:N	2.51	0.44
1:B:265:ASP:OD2	2:B:1444:NAG:H3	2.17	0.44
1:A:278:TYR:HA	1:A:282:VAL:O	2.18	0.44
1:B:301:ARG:HG2	1:B:303:VAL:HG23	1.99	0.43
1:B:265:ASP:HA	1:B:299:THR:CB	2.47	0.43
1:A:266:VAL:HB	1:A:300:TYR:HB2	1.98	0.43
1:B:363:VAL:HG22	1:B:412:VAL:O	2.18	0.43
3:A:2037:HOH:O	1:B:351:LEU:HD22	2.17	0.43
1:B:238:PRO:HB2	1:B:328:LEU:HD13	2.01	0.43
1:A:348:VAL:O	1:A:439:LYS:HG3	2.19	0.43
1:B:278:TYR:HE2	1:B:284:VAL:HG22	1.83	0.43
1:B:414:LYS:O	1:B:418:GLN:HG3	2.18	0.43
1:B:338:LYS:NZ	1:B:430:GLU:OE2	2.52	0.42
1:A:287:ALA:O	1:A:288:LYS:C	2.56	0.42
1:A:384:ASN:CG	1:A:385:GLY:H	2.22	0.42
1:B:368:LEU:HD12	1:B:369:VAL:N	2.34	0.42
1:B:357:GLU:C	1:B:359:THR:H	2.23	0.42
1:B:291:PRO:O	1:B:292:ARG:HB3	2.19	0.42
1:B:266:VAL:HB	1:B:300:TYR:CD2	2.54	0.42
1:A:264:VAL:O	1:A:265:ASP:HB2	2.18	0.42
1:A:394:THR:HA	1:B:397:VAL:HG21	2.02	0.42
1:A:342:GLN:HA	1:A:343:PRO:HD3	1.83	0.42
1:A:386:GLN:HG3	1:A:387:PRO:HD2	2.02	0.42
1:B:296:TYR:OH	1:B:301:ARG:NH1	2.46	0.42
1:A:283:GLN:C	1:A:285:HIS:H	2.23	0.42
1:A:314:LEU:HA	1:A:314:LEU:HD23	1.87	0.42
1:A:369:VAL:HB	1:A:406:LEU:HD12	2.02	0.42
1:A:328:LEU:HA	1:A:329:PRO:HD3	1.94	0.42
1:B:350:THR:HB	1:B:441:LEU:CD1	2.50	0.42
1:A:336:ILE:HG12	1:A:337:SER:N	2.35	0.42
1:B:307:THR:HA	3:B:2017:HOH:O	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:344:ARG:HD2	3:B:2031:HOH:O	2.20	0.41
1:A:367:CYS:HB2	1:A:381:TRP:CH2	2.55	0.41
1:A:391:TYR:C	1:A:391:TYR:CD2	2.92	0.41
1:A:274:LYS:HE2	1:A:324:SER:HB2	2.02	0.41
2:B:1450:MAN:O3	2:B:1451:NAG:C1	2.66	0.41
1:B:335:THR:O	1:B:336:ILE:HB	2.21	0.41
1:A:417:TRP:HH2	1:A:441:LEU:CD2	2.33	0.41
1:B:276:ASN:HB3	1:B:278:TYR:CE1	2.56	0.41
1:B:325:ASN:HD22	1:B:326:LYS:N	2.15	0.41
1:A:328:LEU:HD12	1:A:329:PRO:CD	2.50	0.41
1:B:273:VAL:HB	1:B:302:VAL:HG21	2.03	0.41
1:B:367:CYS:HB2	1:B:381:TRP:CZ2	2.56	0.41
1:B:296:TYR:HE2	2:B:1445:FUL:H2	1.86	0.41
1:B:311:GLN:N	1:B:311:GLN:NE2	2.53	0.41
1:A:238:PRO:HD2	3:A:2002:HOH:O	2.21	0.41
1:B:268:HIS:O	1:B:271:PRO:CG	2.68	0.40
1:B:351:LEU:HB2	1:B:366:THR:HB	2.03	0.40
1:A:394:THR:HG23	1:A:407:TYR:O	2.22	0.40
1:B:350:THR:HB	1:B:441:LEU:CG	2.51	0.40
1:A:439:LYS:HD3	1:A:439:LYS:HA	1.91	0.40
1:A:432:LEU:O	1:A:435:HIS:N	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	206/223 (92%)	175 (85%)	20 (10%)	11 (5%)	3	1
1	B	205/223 (92%)	178 (87%)	17 (8%)	10 (5%)	3	1
All	All	411/446 (92%)	353 (86%)	37 (9%)	21 (5%)	3	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	287	ALA
1	A	289	THR
1	A	433	HIS
1	B	298	SER
1	B	301	ARG
1	A	267	SER
1	A	298	SER
1	B	271	PRO
1	A	293	GLU
1	B	282	VAL
1	B	291	PRO
1	B	293	GLU
1	A	286	ASN
1	A	358	MET
1	A	385	GLY
1	B	283	GLN
1	B	295	GLN
1	B	327	ALA
1	B	336	ILE
1	A	290	LYS

5.3.2   Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/206 (94%)	187 (97%)	6 (3%)	52	73
1	B	192/206 (93%)	180 (94%)	12 (6%)	25	37
All	All	385/412 (93%)	367 (95%)	18 (5%)	36	53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	VAL
1	A	292	ARG
1	A	406	LEU
1	A	413	ASP
1	A	436	TYR

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Mol	Chain	Res	Type
1	A	441	LEU
1	B	255	ARG
1	B	260	THR
1	B	278	TYR
1	B	288	LYS
1	B	291	PRO
1	B	296	TYR
1	B	311	GLN
1	B	370	LYS
1	B	394	THR
1	B	399	ASP
1	B	406	LEU
1	B	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	GLN
1	A	283	GLN
1	A	311	GLN
1	A	325	ASN
1	A	347	GLN
1	A	361	ASN
1	A	390	ASN
1	A	418	GLN
1	A	419	GLN
1	A	421	ASN
1	A	429	HIS
1	B	272	GLN
1	B	276	ASN
1	B	283	GLN
1	B	286	ASN
1	B	311	GLN
1	B	312	ASN
1	B	325	ASN
1	B	342	GLN
1	B	361	ASN
1	B	389	ASN
1	B	390	ASN
1	B	419	GLN
1	B	429	HIS
1	B	434	ASN

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Mol	Chain	Res	Type
1	B	438	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

16 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	NAG	A	1445	1,2	12,14,15	0.51	0	15,19,21	0.97	0
2	FUL	A	1446	2	9,10,11	0.48	0	10,14,16	0.38	0
2	NAG	A	1447	2	12,14,15	0.61	0	15,19,21	0.68	0
2	BMA	A	1448	2	10,11,12	0.44	0	11,15,17	0.50	0
2	MAN	A	1449	2	10,11,12	0.36	0	11,15,17	0.29	0
2	NAG	A	1450	2	12,14,15	0.48	0	15,19,21	0.82	1 (6%)
2	MAN	A	1451	2	10,11,12	0.41	0	11,15,17	0.34	0
2	NAG	A	1452	2	12,14,15	0.51	0	15,19,21	0.65	0
2	NAG	B	1444	1,2	12,14,15	0.58	0	15,19,21	1.01	0
2	FUL	B	1445	2	9,10,11	0.54	0	10,14,16	0.88	0
2	NAG	B	1446	2	12,14,15	0.54	0	15,19,21	0.67	0
2	BMA	B	1447	2	10,11,12	0.41	0	11,15,17	0.59	0
2	MAN	B	1448	2	10,11,12	0.42	0	11,15,17	0.26	0
2	NAG	B	1449	2	12,14,15	0.38	0	15,19,21	0.78	0
2	MAN	B	1450	2	10,11,12	0.58	0	11,15,17	0.53	0
2	NAG	B	1451	2	12,14,15	0.37	0	15,19,21	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1445	1,2	-	0/6/23/26	0/1/1/1
2	FUL	A	1446	2	-	0/0/17/20	1/1/1/1
2	NAG	A	1447	2	-	0/6/23/26	0/1/1/1
2	BMA	A	1448	2	-	0/2/19/22	0/1/1/1
2	MAN	A	1449	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1450	2	-	0/6/23/26	0/1/1/1
2	MAN	A	1451	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1452	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1444	1,2	-	0/6/23/26	0/1/1/1
2	FUL	B	1445	2	-	0/0/17/20	0/1/1/1
2	NAG	B	1446	2	-	0/6/23/26	0/1/1/1
2	BMA	B	1447	2	-	0/2/19/22	0/1/1/1
2	MAN	B	1448	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1449	2	-	0/6/23/26	0/1/1/1
2	MAN	B	1450	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1451	2	1/1/5/7	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1450	NAG	C2-N2-C7	-2.03	119.68	123.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1451	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1451	NAG	C1-C2-N2-C7

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1446	FUL	C1-C2-C3-C4-C5-O5

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	208/223 (93%)	0.28	6 (2%)	49	47	19, 39, 70, 85	0
1	B	207/223 (92%)	0.81	31 (14%)	3	2	17, 49, 100, 100	0
All	All	415/446 (93%)	0.55	37 (8%)	11	9	17, 43, 99, 100	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	HIS	9.1
1	B	300	TYR	7.5
1	B	286	ASN	6.5
1	B	272	GLN	5.6
1	B	284	VAL	4.9
1	B	276	ASN	4.9
1	B	289	THR	4.6
1	B	296	TYR	4.4
1	B	295	GLN	4.4
1	B	240	VAL	4.2
1	B	239	SER	3.9
1	B	299	THR	3.2
1	B	275	PHE	3.2
1	B	266	VAL	3.0
1	B	328	LEU	3.0
1	B	303	VAL	2.9
1	B	327	ALA	2.9
1	B	294	GLN	2.8
1	A	284	VAL	2.8
1	B	241	PHE	2.8
1	B	319	TYR	2.8
1	B	238	PRO	2.7
1	B	291	PRO	2.5
1	B	293	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	263	VAL	2.5
1	A	285	HIS	2.5
1	B	274	LYS	2.5
1	B	273	VAL	2.4
1	B	264	VAL	2.4
1	A	441	LEU	2.4
1	A	327	ALA	2.4
1	B	302	VAL	2.4
1	B	324	SER	2.4
1	A	286	ASN	2.2
1	B	265	ASP	2.2
1	B	326	LYS	2.1
1	A	289	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	1452	14/15	0.21	1.37	77,81,82,82	0
2	NAG	B	1444	14/15	0.37	0.93	98,99,100,100	0
2	NAG	A	1450	14/15	0.18	0.67	57,61,64,64	0
2	NAG	A	1445	14/15	0.20	0.26	46,56,61,62	0
2	FUL	B	1445	10/11	0.32	0.09	98,100,100,100	0
2	NAG	B	1449	14/15	0.22	0.04	77,79,83,83	0
2	MAN	A	1449	11/12	0.16	-0.61	43,47,48,51	0
2	NAG	B	1451	14/15	0.19	-0.74	93,95,96,97	0
2	BMA	A	1448	11/12	0.15	-0.96	45,47,50,55	0
2	NAG	B	1446	14/15	0.25	-1.19	92,97,98,99	0
2	FUL	A	1446	10/11	0.15	-1.49	64,67,69,69	0
2	NAG	A	1447	14/15	0.15	-2.46	42,45,47,48	0
2	BMA	B	1447	11/12	0.18	-2.59	82,85,87,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
2	MAN	B	1448	11/12	0.13	-5.29	78,79,80,80	0
2	MAN	A	1451	11/12	0.18	-	61,64,67,72	0
2	MAN	B	1450	11/12	0.17	-	78,82,85,89	0

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.